Dispersion of confined optical phonons in semiconductor nanowires in the framework of a continuum approach

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Confined optical phonons are discussed for a semiconductor nanowire of the Ge (Si) prototype on the basis of a theory developed some years ago. In the present work this theory is adapted to a non polar material and generalized to the case when the phonon dispersion law involves both linear and quadratic terms in the wave vector. The treatment is considered along the lines of a continuous medium model and leads to a system of coupled differential equations describing oscillations of mixed nature. The nanowire is modelled in the form of an infinite circular cylinder and the solutions of the fundamental equations are found. We are thus led to a description of long wavelength optical phonons, which should show a closer agreement with experimental data and with calculations along atomistic models. The presented theory is applied to the calculation of optical phonons in a Ge nanowire. We have found the dispersion curves for various optical phonon modes. We also normalize the modes and discuss the electron-phonon interaction within the deformation potential approximation.

I. INTRODUCTION

The study of semiconductor nanowires is of current importance both for device applications and fundamental physics, a point that has been recognized since a certain time ago.[1] More recently, the fabrication of Si and Ge nanowires by means of different techniques has been stimulated in view of their relevance in device nanotechnology .[2,3,4,5,6] The physical properties of these nanostructures are being studied both theoretically and experimentally, while the fabrication of field-effect transistors on the basis of this type of systems has been also reported.[7,8,9,10,11,12,13] In the present work we are interested in the phonon properties of non polar nanowires of the Ge and Si prototypes, and, particularly, in the optical phonons. It is well-known that phonon properties play an important role in the considered systems because of their significance for the analysis of various physical processes, such as, charge and thermal transport, optical transitions, etc. Moreover, phononic engineering has been invoked for device application purposes,[14] making it relevant to have a better description of phonon modes.

The analysis of phonon properties in quantum-wires already has a long history. By applying the long-wavelength approximation, based on continuum approaches, the polar optical phonons were discussed by different authors more than a decade ago[15,16,17,18] (see also Ref. 19 for a more recent paper on the subject). Considering the nanowires made of non polar materials, we must remark the existence of a close related subject: phonons in carbon nanotubes,[20,21] an issue revealing outstanding possibilities for present day nanotechnology.

In the case of nanowires of the Ge or Si prototypes the calculation of optical phonons by means of long-wavelength continuum approaches involves interest by itself, and also for applications. In the framework of the present paper we shall support calculations of the optical phonon modes on a phenomenological theory, which was proposed more than a decade ago for the polar optical phonons in the same kind of nanostructures.[22,23,24] Using this approach polar optical phonons in quantum-wires were studied in Refs. 17,18. In the Ref. 21 the same theory, but adapted to non polar optical phonons, was applied to the case of carbon nanotubes. In all the above mentioned works it is explicitly assumed that the optical phonons display a dispersion law quadratic with the wave vector, which, in the bulk semiconductor case is of the form $\omega^2 = \omega_0^2 - \beta^2 k^2$ and, according to this long-wavelength approximation, should be considered near the Γ-point of the Brillouin Zone (BZ).[25] In the present paper the theory is generalized in order to take account of linear terms in the phonon dispersion law, i.e., we assume a more general dispersion law having the form $\omega^2 = \omega_0^2 - \beta' k - \beta^2 k^2$ (in the bulk case). Hence, we propose more general equations that in Ref. 21, now involving linear terms, and also we show how they can be solved. It is easy to realize that the additional linear term allows a better description of the optical phonons near the BZ center, in closer correspondence with both experimental evidence and atomistic calculations involving discretized microscopic models. In some of the studied cases this linear term becomes essential, and this situation is actually realized in nanostructures based on Si and Ge.

Then, the paper is organized as follows. In Section II we present the fundamental equations, discuss their physical meaning and other details of the approach. In Section III we show how the equations can be solved in the case of a wire of circular cross-section and infinite length. Section IV is devoted to a physical discussion of the results obtained, while the case of a Ge nanowire is addressed.

II.   FUNDAMENTAL EQUATIONS

We assume that the relative displacement vector $\boldsymbol{u}$ satisfies the following equation:

$$\rho(\omega^2 - \omega_0^2)\boldsymbol{u} = \rho\beta_L^2\nabla\nabla\cdot\boldsymbol{u} - \rho\beta_T^2\nabla\times\nabla\times\boldsymbol{u} + i\rho(\boldsymbol{a}\cdot\nabla)\boldsymbol{u} + i\rho\boldsymbol{b}(\nabla\cdot\boldsymbol{u}) \ . \tag{1}$$

Equation (1) is analogous to that introduced in Refs. 17,18,22,23,24, just considering that the electric potential is zero (see also Ref. 21). However, new terms were added (two last terms at the r.h.s. of (1)), which modify the nature of the differential equation and lead to the linear terms in the phonon dispersion law. The parameter ρ is the reduced mass density of the two atoms (Ge) in the unit cell, ω_0 is the optical phonon frequency at the Γ point of the bulk semiconductor, and $\boldsymbol{u}(\boldsymbol{r}, t)$ is considered to depend harmonically on the time ($\sim \exp(-i\omega t)$). Parameters β_L and β_T (with dimensions of velocity) are introduced to describe the quadratic (parabolic) phonon dispersion and used to fit the bulk semiconductor dispersion curve. They were already considered in previous works. Now we are introducing new parameters in the form of vectors $\boldsymbol{a}$ and $\boldsymbol{b}$, not considered in previous works and leading to linear terms in the phonon dispersion law. The latter vector parameters are also determined by a fitting of the bulk semiconductor dispersion law for the optical phonons. Equation (1) represents a system of three coupled partial differential equations assumed to describe the confined polar optical phonons in each segment of the semiconductor heterostructure. The solutions must be matched at the interfaces by applying the boundary conditions for $\boldsymbol{u}$, which we shall analyze below.

It is important to notice that all the four terms at the r.h.s. of Eq. (1) may be expressed as the divergence of a tensor σ_{ij}, casted as

$$\sigma_{ij} = \rho(\beta_L^2 - 2\beta_T^2)(\nabla\cdot\boldsymbol{u})\delta_{ij} + \rho\beta_T^2\left(u_{j,i} + u_{i,j}\right) + i\rho\left(b_i u_j + a_j u_i\right) \ . \tag{2}$$

This tensor could be compared to the stress tensor used in the theory of continuous elastic media, and actually its divergence provides a force density. However, in the framework of the present approach, it should be considered as a phenomenological quantity, which is introduced *ad hoc* in order to provide a description of *dispersive* optical phonons in close correspondence with what is seen both experimentally and in atomistic model calculations. In this spirit we do not attempt to explain the tensor σ_{ij} in terms of the elastic properties of the system, and tensor σ_{ij} should not be considered a stress tensor in the strict sense of this concept. The suffixes i, $j = 1$, 2, 3, denoting the cartesian components, should not be confused with the $i = \sqrt{-1}$ used as a factor. Obviously, in all the equations above we assume an isotropic model for the semiconductor. The short notation $u_{i,j}$ denotes the partial derivative with respect to x_j, i. e., $u_{i,j} = \partial u_i/\partial x_j$.

Equations (1) and (2) shall be now applied to the nanowire case, assuming it is an infinite cylinder of circular cross-section with radius r_0. The use of cylindrical coordinates (r, θ, z) becomes a natural choice, and the equations must be written in terms of these coordinates, as well as the tensor σ_{ij}. In the theory of elastic continuous media the standard boundary conditions applied to any interface between two different materials are: (1) continuity of the displacement vector $\boldsymbol{u}$; (2) continuity of the force flux, given by $\sigma \cdot \boldsymbol{N}$, where $\boldsymbol{N}$ is the normal unit vector to this surface. Solutions showing divergences at any point of the region must also be disregarded and, in particular, we must avoid singular solutions in the asymptotic limits $r \to 0, \infty$.

It is convenient to introduce the auxiliary quantities $\boldsymbol{\Gamma} = \nabla\times\boldsymbol{u}$ and $\Lambda = \nabla\cdot\boldsymbol{u}$. Thus, after simple mathematical manipulations, Eq. (1) is transformed into the following equations:

$$\left[\nabla^2 + q_L^2\right]\Lambda \ = \ 0 \ , \tag{3}$$

$$\left[\nabla^2 + q_T^2\right]\boldsymbol{\Gamma} \ = \ \frac{i}{\beta_T^2}\boldsymbol{a}\times\nabla\Lambda \ , \tag{4}$$

where

$$q_L^2 \ = \ \frac{1}{\beta_L^2}\left[\omega_0^2 - \omega^2 + i(\boldsymbol{a}+\boldsymbol{b})\cdot\nabla\right] \ , \tag{5}$$

$$q_T^2 \ = \ \frac{1}{\beta_T^2}\left[\omega_0^2 - \omega^2 + i\boldsymbol{b}\cdot\nabla\right] \ . \tag{6}$$

Notice that the latter quantities are actually differential operators in close correspondence with the starting equation. Another important issue involving Eq. (4) concerns its coupling to Eq. (3). All these features make the differences with respect to previous treatments,[17,18,21] and lead to mathematical complications as a result of our aim of introducing

linear terms in the phonon dispersion law. When applying the equations to the case of an infinite cylinder of radius r_0 filled with an isotropic non polar semiconductor, we may make use of the translational and rotational symmetries of the system, assuming that the solutions must be proportional to $\exp[i(n\theta + kz)]$, where $n = 0, 1, 2, \cdots$ and k plays the role of the wave vector. Moreover, vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ shall be taken along the z-axis, provided that, with this choice, we are led to the appropriate linear dependence on k for the phonon frequencies. Under such conditions $q_{L(T)}^2$ become parameters linearly depending on the wave vector k and given by: $q_L^2 = (\omega_0^2 - \omega^2 - (a+b)k)/\beta_L^2$ and $q_T^2 = (\omega_0^2 - \omega^2 - bk)/\beta_T^2$.

Another point of central importance concerns the boundary conditions that should be applied. In this work we shall consider the nanowire as "free standing", so the appropriate boundary conditions involve zero force at the cylindrical surface of radius r_0. After rewriting tensor σ_{ij} in cylindrical coordinates, and realizing that the normal unit vector $\boldsymbol{N}$ must be taken along the radial direction ($\boldsymbol{N} = \boldsymbol{e}_r$), we should require the components σ_{rr}, $\sigma_{\theta r}$ and σ_{zr} to be equal to zero at $r = r_0$. Starting from Eq. (2), tediously long but straightforward mathematical manipulations lead us to the following results:

$$\sigma_{rr} = \beta_L^2 \frac{\partial u_r}{\partial r} + (\beta_L^2 - 2\beta_T^2)\left(\frac{1}{r}\frac{\partial u_\theta}{\partial \theta} + \frac{\partial u_z}{\partial z} + \frac{1}{r}u_r\right) , \tag{7}$$

$$\sigma_{\theta r} = \beta_T^2 \left(\frac{\partial u_\theta}{\partial r} + \frac{1}{r}\frac{\partial u_r}{\partial \theta} - \frac{1}{r}u_\theta\right) , \tag{8}$$

$$\sigma_{zr} = \beta_T^2 \left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r}\right) + ibu_r . \tag{9}$$

III.   SOLUTION OF THE DIFFERENTIAL EQUATIONS

Assuming $\Lambda(r, \theta, z) = f(r)\exp[i(n\theta + kz)]$, Eq. (3) leads to

$$\frac{d^2 f}{d\xi^2} + \frac{1}{\xi}\frac{df}{d\xi} + \left(1 - \frac{n^2}{\xi^2}\right)f = 0 , \tag{10}$$

where $\xi = Q_L r$ and $Q_L^2 = q_L^2 - k^2$. Eq. (10) is identified as Bessel equation of order n, and its linearly independent (LI) solutions are usually denoted by $J_n(\xi)$ and $Y_n(\xi)$, Bessel functions of the first and second kind, respectively.[26] In our case we shall apply just the function $J_n(\xi)$, convergent in the interior of the cylinder with $0 \le r \le r_0$.

Solutions of Eq. (4), an inhomogeneous Helmholtz equation for the vector quantity Γ, are more difficult to find. In the first place we again shall consider that $\boldsymbol{\Gamma}(r, \theta, z) \sim \exp[i(n\theta + kz)]$. We have found a particular solution of Eq. (4), which is given by

$$\boldsymbol{\Gamma}_P = A\boldsymbol{e}_z \times \nabla\Lambda , \quad \text{with} \quad A = \frac{ia}{\beta_T^2(q_T^2 - q_L^2)} , \tag{11}$$

where $\boldsymbol{e}_z$ is a unit vector along the z-axis.

Then, we just have to find the solution of the homogeneous Helmholtz equation $\boldsymbol{\Gamma}_H$, and the general solution shall be given by $\boldsymbol{\Gamma} = \boldsymbol{\Gamma}_P + \boldsymbol{\Gamma}_H$. As discussed in Ref. 26, page 1766, the two LI solutions of the homogeneous Helmholtz equation for a vector function $\boldsymbol{\Gamma}$, using cylindrical coordinates, are casted as

$$\boldsymbol{\Gamma}_{H1} = \nabla v_1 \times \boldsymbol{e}_z \quad \text{and} \quad \boldsymbol{\Gamma}_{H2} = q_T v_2 \boldsymbol{e}_z + \frac{1}{q_T}\nabla\frac{\partial v_2}{\partial z} , \tag{12}$$

where the functions v_i ($i = 1, 2$) satisfy the scalar homogeneous Helmholtz equations $(\nabla^2 + q_T^2)v_i = 0$, with solutions analogous to those of Λ. After the general solutions for Λ and $\boldsymbol{\Gamma}$ are found, we can find the corresponding solution of Eq. (1) for $\boldsymbol{u}$, which shall be obtained from

$$\boldsymbol{u} = \frac{1}{q_T^2}\left[\nabla \times \boldsymbol{\Gamma} - \left(\frac{\beta_L}{\beta_T}\right)^2 \nabla\Lambda - \frac{ia}{\beta_T^2}\Lambda\boldsymbol{e}_z\right] . \tag{13}$$

In the foregoing calculations the involved mathematical steps are long and tedious, but here we shall report just final expressions. We write $\boldsymbol{u} = \boldsymbol{F}(r)\exp[i(n\theta + kz)]$ where $\boldsymbol{F} = F_r \boldsymbol{e}_r + F_\theta \boldsymbol{e}_\theta + F_z \boldsymbol{e}_z$ and $\boldsymbol{e}_r$, $\boldsymbol{e}_\theta$, and $\boldsymbol{e}_z$, are the unit vectors of the cylindrical coordinates. Then, we have

$$F_r(r) \;=\; J_n'(Q_L r)C_1 + \frac{ik}{Q_T}J_n'(Q_T r)C_2 + \frac{in}{Q_T r}J_n(Q_T r)C_3\,, \tag{14}$$

$$F_\theta(r) \;=\; \frac{in}{Q_L r}J_n(Q_L r)C_1 - \frac{nk}{Q_T^2 r}J_n(Q_T r)C_2 - J_n'(Q_T r)C_3\,, \tag{15}$$

$$F_z(r) \;=\; \frac{i(k-\gamma)}{Q_L}J_n(Q_L r)C_1 + J_n(Q_T r)C_2\,, \tag{16}$$

where $Q_T^2 = q_T^2 - k^2$ and $\gamma = a/(\beta_T^2 - \beta_L^2)$. The "prime" in the Bessel function denotes the first derivative with respect to the function's argument and the constants C_i ($i = 1,\,2,\,3$) should be determined after application of the boundary conditions. As it was already remarked in Section II, we consider a "free standing" wire, and the boundary conditions read as

$$\sigma_{rr}|_{r_0} = 0\,, \quad \sigma_{\theta r}|_{r_0} = 0, \quad \sigma_{zr}|_{r_0} = 0\,, \tag{17}$$

indicating that the internal flux of forces through the boundary surface is zero. Taking Eqs. (7), (8), (9), and (17) into account we are lead to the following system of linear homogeneous equations

$$\sum_{j=1}^{3} G_{ij}C_j = 0\,, \tag{18}$$

where the nine coefficients G_{ij} are explicitly given in the Appendix. The dispersion relations, determining the frequencies of the various phonon modes as functions of the wave vector k, are obtained after solution of the secular equation

$$\det\left[G_{ij}\right] = 0\,, \tag{19}$$

while the components of the vector $\boldsymbol{F}$ are given as

$$F_r(r)/C \;=\; S_1 J_n'(Q_L r) + \frac{ik}{Q_T}S_2 J_n'(Q_T r) + \frac{in}{Q_T r}S_3 J_n(Q_T r)\,, \tag{20}$$

$$F_\theta(r)/C \;=\; \frac{in}{Q_L r}S_1 J_n(Q_L r) - \frac{nk}{Q_T}S_2 \frac{1}{Q_T r}J_n(Q_T r) - S_3 J_n'(Q_T r)\,, \tag{21}$$

$$F_z(r)/C \;=\; \frac{i(k-\gamma)}{Q_L}S_1 J_n(Q_L r) + S_2 J_n(Q_T r)\,, \tag{22}$$

where the functions S_i ($i = 1,\,2,\,3$) are given in the Appendix.

IV. NORMALIZATION OF THE PHONON STATES

The determination of the constant C is made by normalization of the oscillation modes, which requires to transform the classical field $\boldsymbol{u}$ into a quantum-field operator. This is formally done in the form $\boldsymbol{u} \rightarrow \hat{\boldsymbol{u}} = \boldsymbol{u}\hat{a}_{n,\,k}$, where $\hat{a}_{n,\,k}$ are second quantization bosonic operators. Operator $\hat{a}_{n,\,k}$ ($\hat{a}_{n,\,k}^{\dagger}$) annihilates (creates) a "n, k" optical phonon. We must also transform the classical kinetic energy for the oscillations to a quantum-mechanical operator by applying the rule

$$W_{kin} = \frac{1}{2}\rho \int_V \dot{\boldsymbol{u}}^* \cdot \dot{\boldsymbol{u}}\, d^3 r = \frac{1}{2}\rho\omega^2 \int_V \boldsymbol{u}^* \cdot \boldsymbol{u}\, d^3 r \;\rightarrow\; \hat{H}_{ph}\,, \tag{23}$$

where

$$\hat{H}_{ph} = \frac{1}{4}\rho\omega^2 \int_V \left(\hat{\boldsymbol{u}}^\dagger \cdot \hat{\boldsymbol{u}} + \hat{\boldsymbol{u}} \cdot \hat{\boldsymbol{u}}^\dagger\right) d^3r = \frac{1}{2}\rho\omega^2 \int_V \boldsymbol{u}^* \cdot \boldsymbol{u}\, d^3r \left(\hat{a}^\dagger_{n,k}\hat{a}_{n,k} + \frac{1}{2}\right)\ . \tag{24}$$

In Eq. (24) $\hat{H}_{ph}$ describes the free phonons hamiltonian operator, while its hermitian character is ensured by construction. Requiring the latter expression to be given in standard form for phonons of the type "n,k" (actually, we must have $\omega \to \omega_{nk}$) $\hat{H}_{ph} = \hbar\omega_{n,k}\left(\hat{a}^\dagger_{n,k}\hat{a}_{n,k} + \frac{1}{2}\right)$, one can finally write the normalization constant C by

$$C_{n,k} = \sqrt{\frac{\hbar}{\pi L\rho\omega_{n,k}M_{n,k}}}\ , \tag{25}$$

where L is a normalization length (taken along the z axis) and $M_{n,k} = \int(F_r^*(r)F_r(r) + F_\theta^*(r)F_\theta(r) + F_z^*(r)F_z(r))r\,dr/|C_{n,k}|^2$. The explicit expressions for $M_{n,k}$ involve rather complicated integrations of the Bessel functions and may be calculated numerically for each value of k and ω corresponding to the possible oscillation modes.

For optical phonons in a non polar semiconductor the electron-phonon hamiltonian is given through the deformation potential approximation and, for an isotropic semiconductor, is proportional to $\nabla \cdot \boldsymbol{u}$. Then, it is interesting to discuss this latter quantity, which provides an estimative of the interaction strength.

V. DISCUSSION OF RESULTS

With the aim of illustrating the foregoing theory, we consider a Ge nanowire. The Ge physical parameters are given in Table I.

TABLE I: Ge parameters

material	$a_0[10^{-8}cm]$	$\rho\,[g/cm^3]$	$\omega_0\,[cm^{-1}]$	$\beta_T\,[10^5cm/s]$	$\beta_L\,[10^5cm/s]$	$a[10^{18}cm/s^2]$	$b[10^{18}cm/s^2]$
Ge	5.66	5.32	305	3.48	3.55	-6.26	3.59

The parameters β_T, β_L, a and b were determined by the authors by a fitting of the bulk semiconductor phonon dispersion law reported in Ref.27, considering dispersion along the (001) direction and embracing approximately $50-40$ % of the BZ near the Γ point. Parameter ω_0 was taken from the same reference, while the other parameters can be found in Ref. 28.

In Fig. 1 we depict the dispersion relation for several axis-symmetric modes ($n = 0$) taking $r_0 = 10^{-7}$ cm. The frequency is in units of cm^{-1}) and the wave vector k is in units of $2\pi/a_0$, where a_0 is the lattice parameter for the bulk semiconductor). The curves were obtained from Eq. (19) taking $n = 0$. Let us emphasize that these modes do not present torsional oscillations, and they result from a combination of radial breathing vibrations together with vibrations along the cylinder axis (axial oscillations). The latter oscillations are not purely longitudinal as it is sometimes argued, but a mixture of LO and TO oscillations. However, at $k = 0$ the axis-symmetric oscillations separate into pure LO and TO vibrations, a fact we have used for the labelling of the different modes.

Notice that for the curves corresponding to the modes TO$_2$ and LO$_3$ there is an interval of k values (approximately between 0.5 and 0.63) where the curves are interrupted, and no frequencies are reported. This region obviously corresponds to an anticrossing of the mentioned modes. Of course, in the real case, there must be oscillation frequencies and the interrupted curves may be interpreted as a limitation of our approach, which is not able to describe such oscillation modes. However, it is worth to mention that the observed failure has nothing to due with the anticrossing effect by itself. The theory we are applying is essentially valid not too far from the $k = 0$ region, and we are actually extrapolating it beyond this region. This latter issue should be seen as a singular failure of the applied treatment, which, otherwise is giving a rather good description of the dispersion law for these modes. We have set $r_0 = 10^{-7}$ cm, a relatively small radius which, however, is typical for this kind of nanowires. For such thin nanowire the number of physically possible optical phonon modes is rather limited and, in fact, Fig. 1 displays a few more modes than actually present. In the framework of the current paper one important contribution is to stress the importance of taking the role of the linear term into account we have added to our equations. It is easy to convince ourselves of this latter issue: making the linear terms equal to zero the general structure of the dispersion law depicted in Fig. 1 is
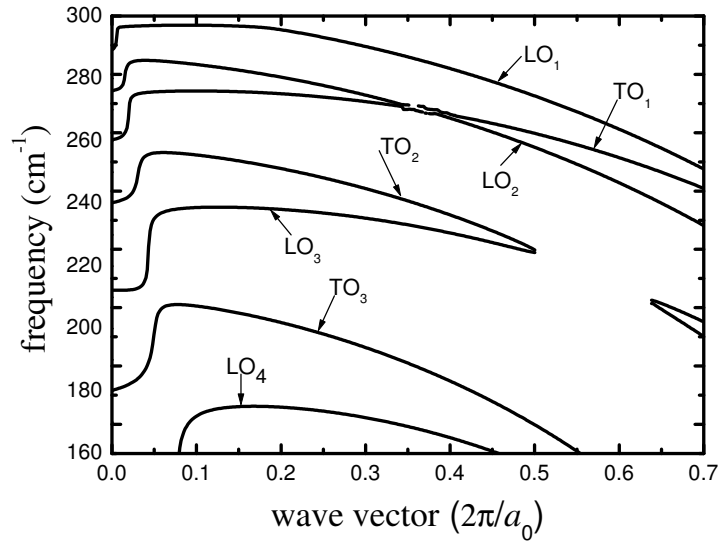
FIG. 1: Dispersion curves for the axis-symmetric modes (n=0). The frequency is in units of cm^{-1} and the wave vector k in units of $2\pi/a_0$) and we take $r_0 = 10^{-7}$ cm.
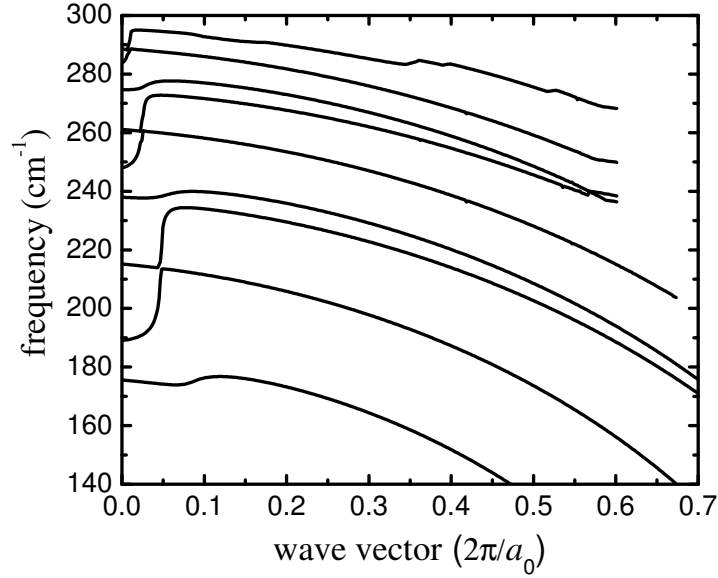

FIG. 2: Dispersion curves for the flexural modes for $n = 1$ taking $r_0 = 10^{-7}$ cm. The frequency is in units of cm^{-1}) and the wave vector k in units of $2\pi/a_0$).

subjected to significant changes. The other interesting point is to compare with experimental results or calculations based upon microscopic (atomistic) approaches. Unfortunately, in the revised literature we have not found reports on optical phonons for this particular type of Ge nanowires.

In Fig. 2 we show the dispersion curves for the so-called flexural modes taking again $r_0 = 10^{-7}$ cm and for $n = 1$. These modes involve all kinds of possible vibrations: radial, axial and torsional. Torsional modes can be considered for any $n > 0$ and we are analyzing the case with $n = 1$. In the chosen frequency interval ($140 < \omega < 300$ cm^{-1}), involving the higher frequency values, just nine modes are present. We should remark that, for the flexural modes, the oscillations have always a mixed character and cannot be separated into pure LO and TO oscillations. In contrast with the axis-symmetric modes the mixing is present even at $k = 0$, and then we cannot classify the modes in the same way as we did in Fig. 1. Other feature clearly seen in Fig. 2 is the presence of several anticrossing regions: curves belonging to the same symmetry cannot cross each other and are "repelled" whenever they get too close. Finally, there are several curves (those with the higher frequencies) that are interrupted for the higher values of k (especially,
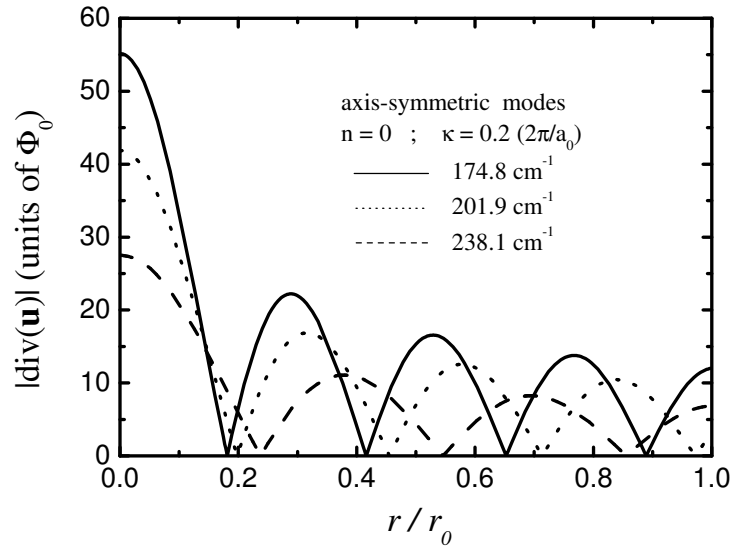
FIG. 3: Absolute value of the divergence of vector $\boldsymbol{u}$ (in units of Φ_0) as a function of r/r_0 for the axis-symmetric modes ($n = 0$). We fixed $k = 0.2(2\pi/a_0)$ and considered the frequencies 174.8, 201.9 and 238.1 cm^{-1} corresponding to three possible modes displayed in Fig. 1.
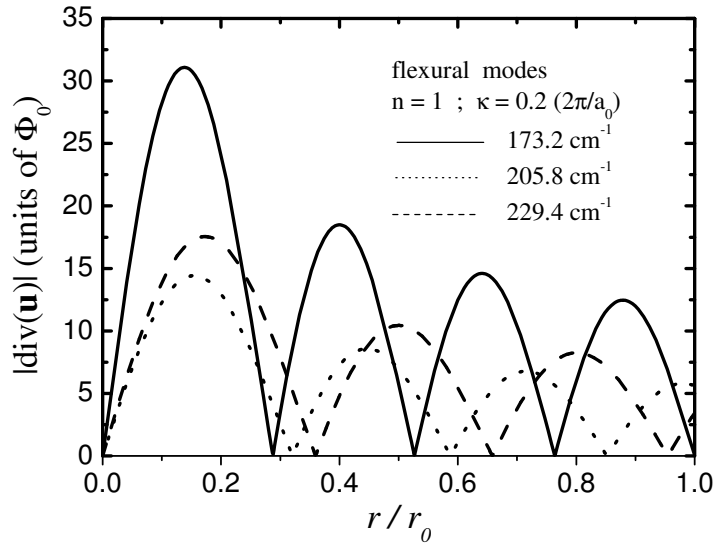

FIG. 4: Absolute value of the divergence of vector $\boldsymbol{u}$ (in units of Φ_0) as a function of r/r_0 for the flexural modes ($n = 1$). We fixed $k = 0.2(2\pi/a_0)$ and considered the frequencies 173.18, 205.8 and 229.4 cm^{-1} corresponding to three possible modes displayed in Fig. 2.

in the region $k > 0.6$, in units of $2\pi/a_0$). The explanation for this effect is the same as in Fig. 1: a failure of the used approximation, which is actually valid for values of k not too far from $k = 0$. However, we must again remark that the theory actually gives a very useful description of the considered modes for a relatively wide interval of k ($60 - 70$ % of the BZ).

Besides the dispersion curves, we find interesting to analyze the quantity given by $\nabla \cdot \boldsymbol{u} \equiv div\,(\boldsymbol{u})$, as a function of r in the interval $r \leq r_0$. The point is that this quantity is proportional to the electron-phonon interaction according to the *deformation potential* approximation, and then can give us an estimative of the strength of this interaction. We have taken the divergence of vector $\boldsymbol{u}$, given in Eq. (22) in cylindrical coordinates, together with the normalization constant, Eq. (25), which was evaluated numerically.

In Fig. 3 we plot the absolute value of the mentioned quantity ($|div\,(\boldsymbol{u})|$) in units of $\Phi_0 = [\hbar/L\rho\pi\omega_0 r_0^4]^{(1/2)}$ as a function of r/r_0. We show three curves corresponding to the axis-symmetric modes ($n = 0$) with a fixed value of k

($k = 0.2(2\pi/a_0)$ and three possible frequencies ($\omega = 174.8$, 201.9, 238.1 cm^{-1}) involving three different modes (the modes LO_4, TO_3, and LO_3 respectively). In Fig. 3 the oscillatory behavior of the interaction potential strength is seen, a clearly understandable fact if we realize that it is given as a combination of Bessel functions. At the point $r = 0$ the quantity is not zero, while the points of maxima determine the values of r where the interaction strength should be stronger. Moreover, for the modes with increasing values of the frequency the strength of the interaction gets weaker. When plotting the absolute value of $div\,(\boldsymbol{u})$ we have lost all information concerning its dependence with respect to θ and z. However, we retained the important information about its r dependence. In should also be kept in mind that, in order to obtain a better estimation of the electron-phonon interaction strength, it is necessary to evaluate the corresponding matrix elements involving the electron wave functions. If the electron wave function is peaked at a point where the deformation potential has a low value, we should realize that the interaction strength still may be strong depending on the relative weight of both effects. The plot displayed in Fig. 4 is quite similar to that of Fig. 3, but now considering the $n = 1$ case (flexural modes). We again see the oscillatory behavior for the same reason as in Fig. 3, but now the involved quantity is zero at $r = 0$, and the calculated strengths are somewhat lower. It is also seen that the deformation potential is not lower for higher values of the frequency. In fact, the intermediate frequency mode leads to weaker intensities that the lower frequency mode. The same comments as those done for Fig. 3 can be made.

In conclusion, we have calculated the optical phonon modes for a Ge nanowire in the framework of a continuum approach. The applied theoretical treatment was adapted to the non polar case, and also was improved by incorporating the important linear terms in the wave vector. In this context we expect the theory to provide better results than those given by other long wavelength treatments. But, as was already remarked, we do not presently have experimental results or microscopic atomistic calculations allowing a desirable comparison with our findings. Nevertheless, and due to the current interest in the study of this kind of nanostructures, we think the results of the present work should be useful in the way to get a better understanding of Ge and Si nanowires.

Appendix A.

The nine functions G_{ij}, appearing in Eq. (18), are given in the form

$$
\begin{aligned}
G_{11} &= \beta_L^2 Q_L \left\{ \left[\left(\frac{\beta_T n}{\beta_L \eta} \right)^2 - \left(1 - \left(\frac{\beta_T}{\beta_L} \right)^2 \right) \nu(\nu - \alpha)/\eta^2 - 1 \right] J_n(\eta) - 2 \left(\frac{\beta_T}{\beta_L} \right)^2 J_n'(\eta)/\eta \right\}, \\
G_{12} &= \frac{2ik\beta_T^2}{\mu^2} \left[(n^2 - \mu^2) J_n(\mu) - \mu J_n'(\mu) \right], \\
G_{13} &= -\frac{2in\beta_T^2 Q_T}{\mu^2} \left[J_n(\mu) - \mu J_n'(\mu) \right], \\
G_{21} &= -\frac{2in\beta_T^2 Q_L}{\eta^2} \left[J_n(\eta) - \eta J_n'(\eta) \right], \\
G_{22} &= \frac{2nk\beta_T^2}{\mu^2} \left[J_n(\mu) - \mu J_n'(\mu) \right], \\
G_{23} &= \frac{\beta_T^2 Q_T}{\mu^2} \left[2\mu J_n'(\mu) + (\mu^2 - 2n^2) J_n(\mu) \right], \\
G_{31} &= i\beta_T^2 k \left[2 - \alpha/\nu + br_0/(\beta_T^2 \nu) \right] J_n'(\eta), \\
G_{32} &= -\frac{\beta_T^2 k^2}{Q_T} \left[1 - (\mu/\nu)^2 + br_0/(\beta_T^2 \nu) \right] J_N'(\mu), \\
G_{33} &= -\frac{nk\beta_T^2}{\mu} \left[1 + br_0/(\beta_T^2 \nu) \right] J_n(\mu),
\end{aligned}
\tag{A1}
$$

where $\alpha = \gamma r_0$, $\nu = k r_0$, $\eta = Q_L r_0$, and $\mu = Q_T r_0$. On the other hand, the functions S_i, present in Eqs. (20), (21) and (22), are defined as

$$
\begin{aligned}
S_1 &= G_{32} G_{23} - G_{22} G_{33}, \\
S_2 &= G_{21} G_{33} - G_{31} G_{23}, \\
S_3 &= G_{31} G_{22} - G_{32} G_{21}.
\end{aligned}
\tag{A2}
$$

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[1] A. P. Alivisatos, Science **271**, 933 (1996).

[2] M. Kawamura, N. Paul, V. Cherepanov, and B. Voigtländer, Phys. Rev. Lett. **91**, 96102 (2003).

[3] Y. F. Zhang, Y. H. Tang, N. Wang, C. S. Lee, I. Bello, and S. T. Lee, Phys. Rev. B **61** , 4518 (2000).

[4] J. H. He, T. H. Wu, C. L. Hsin, L. J. Chen, and Z. L. Wang, Electrochem. and Solid-State Lett. **8**, G254 (2005).

[5] D. Erts, B. Polyakov, E. Saks, H. Olin, L. Ryen, K. Ziegler, and J. D. Holmes, Solid State Phenomena, Vols. **99-100**, 109 (2004).

[6] G. Gu, M. Burghard, G. T. Kim, G. S. Düsberg, P. W. Chiu, and W. Q. Han, J. of Appl. Phys. **90** 5747 (2001).

[7] C. Dames and G. Chen, J. Of Appl. Physics **95**, 682 (2004).

[8] A. B. Greytak, L. J. Lauhon, M. S. Gudiksen, and Ch. M. Lieber, Appl. Phys. Lett. **84**, 4176 (2004).

[9] S. C. Jain, K. Pinardi, H. E. Maes, R. van Overstraeten, A. Atkinson, and M. Willander, Semicond. Sci. Technol. **12** 1507 (1997).

[10] K. W. Adu, H. R. Gutiérrez, U. J. Kim, G. U. Sumanasekera, and P. C. Eklund, Nanoletters **5**, 409 (2005).

[11] E. P. Pokatilov, V. A. Fonoberov, S. N. Balaban, and V. M. Fomin, J. Phys.: Condens, Matter **12**, 9037 (2000).

[12] D. Wang, A. Javey, R. Tu, H. Dai, H. Kim, P. McIntyre, T. Krishnamohan, and K. Saraswat, Appl. Phys. Lett. **83**, 2432 (2003).

[13] M. J. Rack, T. J. Thorton, and D. K. Ferry, Superlattices and Microstructures **28**, 369 (2000).

[14] A. A. Balandin, J. of Nanoscience and Nanotechnology, **5**, 1 (2005).

[15] M. A. Stroscio, K. W. Kim, M. A. Littlejohn, and H. Huang, Phys. Rev. B **42**, 1488 (1990).

[16] R. Enderlein, Phys. Rev. B **47**, 2162 (1993).

[17] F. Comas, C. Trallero-Giner, and A. Cantarero, Phys. Rev. B **47**, 7602 (1993).

[18] F. Comas, A. Cantarero, C. Trallero-Giner, and M. Moshinsky, J. Phys.: Condens. Matter **7**, 1789 (1995).

[19] G. D. Mahan, R. Gupta, Q. Xiong, C. K. Adu, and P. C. Eklund, Phys. Rev. B **68**, 73402 (2003).

[20] M. A. Stroscio, M. Dutta, D. Kahn, and K. W. Kim, Superlattices and Microstructures **29**, 369 (2001).

[21] L. Chico and R. Pérez-Alvarez, Phys. Rev. B **69**, 35419 (2004).

[22] F. Comas and C. Trallero-Giner, Physica B **192**, 394 (1993).

[23] C. Trallero-Giner and F. Comas, Phil. Magazine B, **70**, 583 (1994).

[24] C. Trallero-Giner, R. Pérez, and F. García-Moliner, *Long wave polar optical modes in semiconductor heterostructures*, (Pergamon Press, London, 1998).

[25] In this formula ω is the frequency (in units of rad/s), k is the wave vector, β a phenomenological parameter used to fit the experimentally reported bulk semiconductor dispersion law for the phonons near the point $k = 0$ of the BZ. Obviously, ω_0 is the phonon frequency at $k = 0$.

[26] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics*, (MacGraw-Hill, NY, 1953).

[27] W. Weber, Phys. Rev. B **15**, 4789 (1977).

[28] E. Kasper and F. Schäffler in *Semiconductors and Semimetals, Vol. 33*, ed. T. P. Pearsall (Academic Press, NY, 1991), p. 223.